Research Internship for 2016

Laboratory:
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Theoretical study of thermal and thermoelectric properties of polytypes Ge nanowires

Scientific Context

An internship position is available in the COMputationnal electronICS group and is aimed to investigate theoretically the electronic and thermal properties of new kind of Ge nanowires, recently synthetized in the lab. By applying a powerful combination of quantum-mechanical theory and computer simulation, the work will be carried out in strong collaboration with experimentalists. Nanowires have acquired in the last years a prominent role in several cutting-edge research topics in nanoscience such as electronics, optoelectronics and renewable energy (photovoltaics and thermoelectrics) thanks to their unique electronic and thermal properties and compatibility with the existing microelectronic technology.

Among various parameters characterizing a nanowire (such as size, composition, geometry, etc.), recently the polytype has emerged as an important aspect of investigation. Polytypism is a one-dimensional variant of the well known phenomena of polymorphism, i.e. the ability of a solid material to exist in more than one form or crystal structure [1]. In our lab, the Heterna group has recently developed an experimental method to achieve an unexpected martensitic phase transformation in Ge nanowires under external stress [2]. Though hexagonal Ge were observed 30 years ago [3.], its structure and physical properties remain widely unexplored a deep investigation of the transport properties of novel Ge nanowires polytypes is needed to evaluate the actual potential for technological applications. Both theoretical and experimental investigations are needed to understand the specific behavior of such particularly appealing structure.

Methodology and objectives

As the Fourier heat equation does not rigorously describe the thermal transport at the nanoscale, we develop a home-made device simulator based on a particle Monte Carlo approach dedicated to this specific Ge Nanowire. The student in internship will have 3 objectives:

- **(i)** Using the available code to study the thermal transport,
- **(ii)** Making comparison between theoretical and experimental results,
- **(iii)** Developing the coupling between heat and electron transport.

This work will be developed under the support of the nanodesign plateform of the Université Paris Saclay.

Skills learned during the thesis

The student will acquire a broad range of skills: in solid state physics (band structure, phonon spectrum, electron transport, electron-phonon interaction and phonon-phonon interaction), technology devices, and scientific programming (Fortran and / or C / C + +, Matlab).

Candidate's Profile

Successful candidates must have a MSc in Physics, Electronics, Materials Science or related disciplines. We are seeking creative and highly motivated individuals well trained and skilled in scientific research, and available to collaborate in an interdisciplinary team. Programming experience is also desirable, but not mandatory.

Please join a CV, a list of courses that you have followed and results of exams in the framework of your master program, and any other information that you judge useful.

References:

[1] A.R. Verma and P. Krishna, Polymorphism and Polytypism in Crystals, Wiley, New York (1966).
[2] L. Vincent, et al., Novel Heterostructured Ge Nanowires Based on Polytype Transformation, Nano Lett., 14 (8), pp 4828–4836 (2014)
[3] R.H. Wentorf and J.S. Kasper, Science 139, 238 (1962)